

# **Contribution of regional-scale fire events to ozone and PM2.5 air quality estimated by photochemical modeling approaches**

## **Supporting Information**

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Table S-1. CMAQ v5.0.2 aerosol species, density assumption, visual index factor, and optical surrogate. See Table S-2 for refractive index associated with the optical surrogate name.

Aitken	Accum	Coarse	Density (kg/m3)	Visual Index Factor	Optical Surrogate Name	File Emissions Name
ASO4I	ASO4J	ASO4K	1800	3	SOLUTE	PSO4
ANO3I	ANO3J	ANO3K	1800	3	SOLUTE	PNO3
ACLI	ACLJ	ACKL	2200	0	SOLUTE	PCL
ANH4I	ANH4J	ANH4K	1800	3	SOLUTE	PNH4
ANAI	ANAJ		2200	0	SOLUTE	PNA
	AMGJ		2200	1	DUST	PMG
	AKJ		2200	1	DUST	PK
	ACAJ		2200	1	DUST	PCA
APOCI	APOCJ		2000	4	BCARBO	POC
APNCOMI	APNCOMJ		2000	4	BCARBO	PNCOM
AECI	AECJ		2200	10	SOOT	PEC
	AFEJ		2200	1	DUST	PFE
	AALJ		2200	1	DUST	PAL
	ASIJ		2200	1	DUST	PSI
	ATIJ		2200	1	DUST	PTI
	AMNJ		2200	1	DUST	PMN
AH2OI	AH2OJ	AH2OK	1000	0	WATER	PH2O
AOTHRI	AOTH RJ		2200	1	DUST	PMOTHR
	AALKJ		2000	4	DUST	
	AXYL1J		2000	4	DUST	
	AXYL2J		2000	4	DUST	
	AXYL3J		2000	4	DUST	
	ATOL1J		2000	4	DUST	
	ATOL2J		2000	4	DUST	
	ATOL3J		2000	4	DUST	
	ABNZ1J		2000	4	DUST	
	ABNZ2J		2000	4	DUST	
	ABNZ3J		2000	4	DUST	
	ATRP1J		2000	4	DUST	
	ATRP2J		2000	4	DUST	
	AISO1J		2000	4	DUST	
	AISO2J		2000	4	DUST	
	AISO3J		2000	4	DUST	
	ASQTJ		2000	4	DUST	
	AOLGAJ		2000	4	DUST	
	AOLGBJ		2000	4	DUST	
	AORGJ		2000	4	DUST	
	ASOIL		2600	0	DUST	
	ACORS		2200	0	DUST	PMC
	ASEACAT		2200	0	SOLUTE	

Table S-2. CMAQ v5.0.2 refractive index table for the sensitivity (top) and baseline (bottom) simulation. The values are dimensionless. The imaginary component indicates how much the medium attenuates light. The real component indicates how the medium affects the wavelength and speed relative to how much the medium refracts or bends light's path.

SENSITIVITY	Real Part			Imag Part			
	Name	I	J	K	I	J	K
SOLUTE	1.53	1.53	1.53		0	0	0
SEASALT	1.51	1.51	1.51		0	0	0
BCARBO	1.76	1.76	0		0.02	0.02	0.02
DUST	1.53	1.53	1.53		0.01	0.01	0.01
WATER	1.36	1.36	1.36		0	0	0
SOOT	1.85	1.85	0		0.71	0.71	0

\*The above values for soot-like particles are modified from Table 1 of Horvath 1995. They are size dependent (for I, J, and K modes) effective refractive indices fit to data on absorption by carbon.

\*Water soluble values are modeled on data from Beyer et al. 1996.

\*The values for soot reflect recommendations from Bond (2012), Bond and Bergstrom (2006), and Chang et al. (1990).

BASELINE	Real Part			Imag Part			
	Name	I	J	K	I	J	K
SOLUTE	1.5	1.5	1.5		0	0	0
SEASALT	1.5	1.5	1.5		0	0	0
BCARBO							
DUST	1.53	1.53	1.53		0.01	0.01	0.01
WATER	1.34	1.34	1.34		0	0	0
SOOT	1.53	1.53	0	0	0.14	0.05	0

\*The above values for soot-like particles are modified from Table 1 of Horvath 1995. They are size dependent (for I, J, and K modes) effective refractive indices fit to data on absorption by carbon.

\*Water soluble values are modeled on data from Beyer et al. 1996.

Table S-3. Model performance metrics for O<sub>3</sub>, PM<sub>2.5</sub> sulfate ion, PM<sub>2.5</sub> nitrate ion, PM<sub>2.5</sub> organic carbon, and PM<sub>2.5</sub> elemental carbon across all sites in the model domain during the Wallow fire period and Flint Hills fire period. Hourly ozone estimates are matched with CASTNET monitors. Daily average speciated PM<sub>2.5</sub> estimates are matched with IMPROVE monitors. This performance evaluation has not been subset in any way to match times and locations impacted by fires. This performance evaluation is intended only to provide context for the surrounding environment of the fires modeled here.

Modeling Time Period	Pollutant	Units	N	Mean Bias	Mean Error	Median Bias	Median Error
Wallow Period	O3	ppb	9,984	-2.20	10.50	-1.90	8.10
	PM2.5 SO4	ug/m <sup>3</sup>	260	-0.33	0.50	-0.12	0.23
	PM2.5 OC	ug/m <sup>3</sup>	267	-0.59	1.03	-0.40	0.49
	PM2.5 NO <sub>3</sub>	ug/m <sup>3</sup>	257	-0.11	0.19	-0.11	0.14
	PM2.5 EC	ug/m <sup>3</sup>	268	0.04	0.18	-0.01	0.06
Flint Hills Period	O3	ppb	23,539	-2.60	7.60	-2.90	6.10
	PM2.5 SO4	ug/m <sup>3</sup>	532	-0.03	0.39	0.05	0.22
	PM2.5 OC	ug/m <sup>3</sup>	552	0.17	0.58	0.01	0.16
	PM2.5 NO <sub>3</sub>	ug/m <sup>3</sup>	532	0.05	0.31	-0.04	0.13
	PM2.5 EC	ug/m <sup>3</sup>	554	0.09	0.14	0.02	0.04

Model performance metrics used to compare observations and model predictions:

Mean Bias	
Mean Error	
Median Bias	Median(model-observed)
Median Error	Median(absolute(model-observed))

Figure S-1a. Model domain extent and daily centroid location of modeled Wallow and Flint Hills fires included in this model assessment.



Figure S-1b. Daily centroid location of modeled Wallow and Flint Hills fires included in this model assessment. Routine surface monitors used in the fire impact evaluation are also shown.

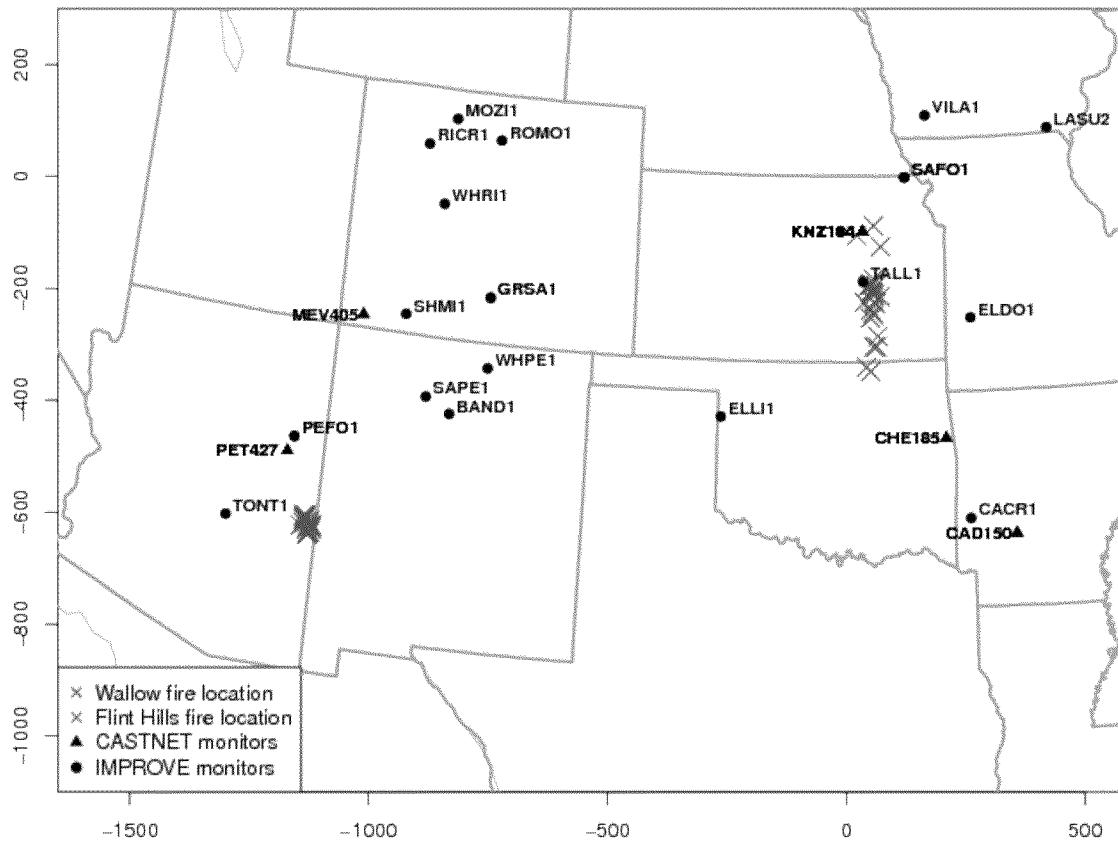


Figure S-2. Temporal profile used for wild and prescribed fire types to allocate daily emissions to hour of the day. These profiles represent the average at each hour of fractional allocation that varies slightly by State.

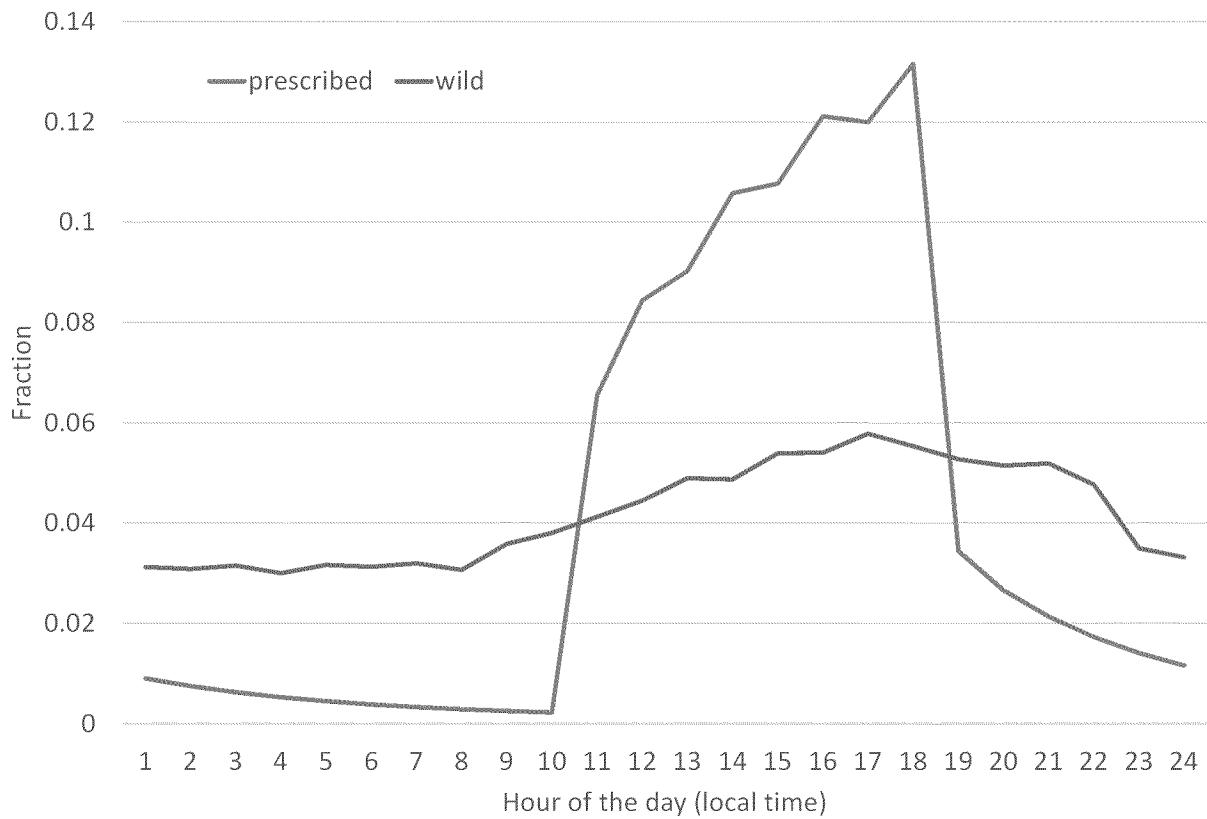


Figure S-3. HMS plots for the Wallow fire modeling period in June 2011. The HMS product is a column total smoke density and does not provide an estimate of surface layer O<sub>3</sub> or PM<sub>2.5</sub> impacts.

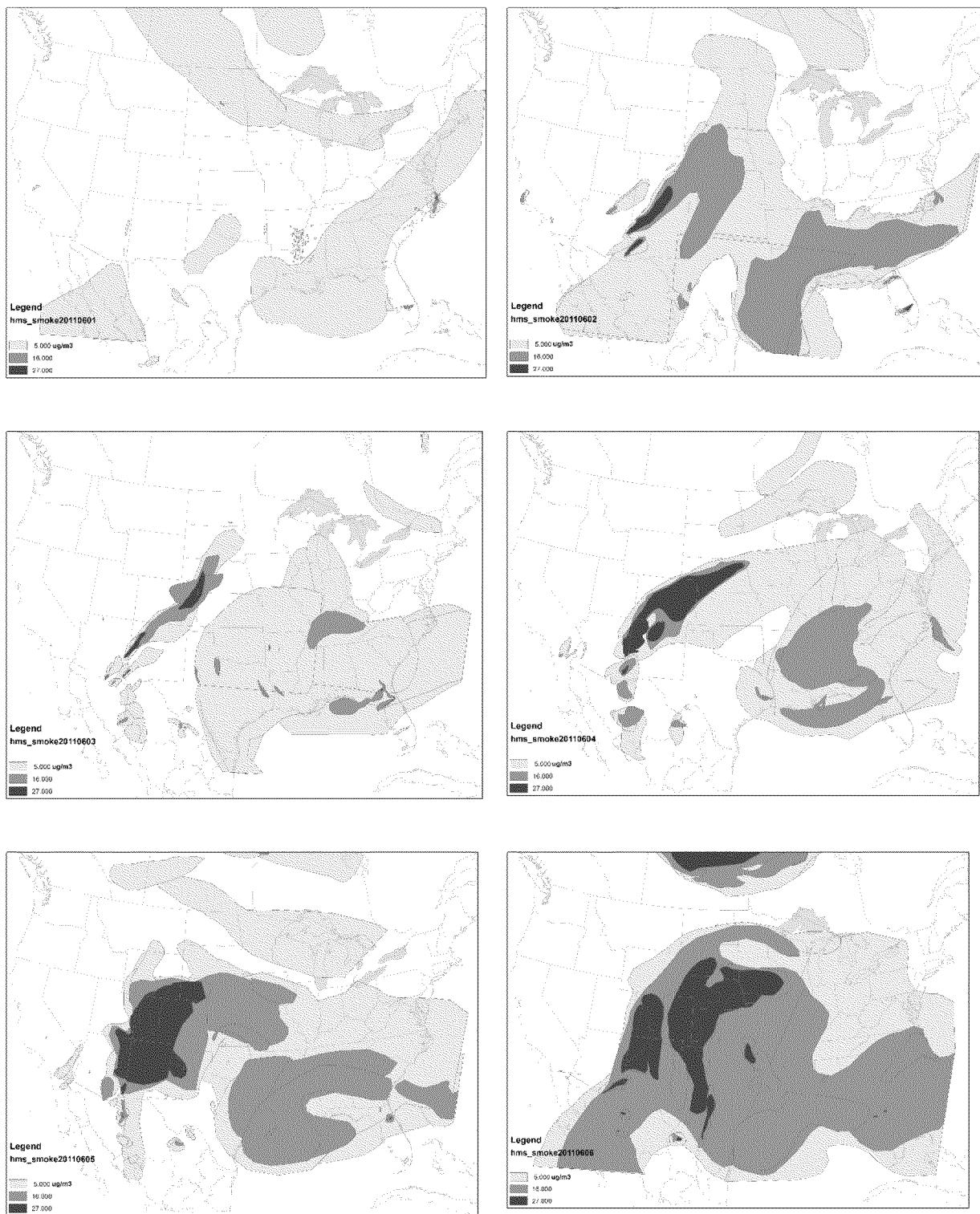
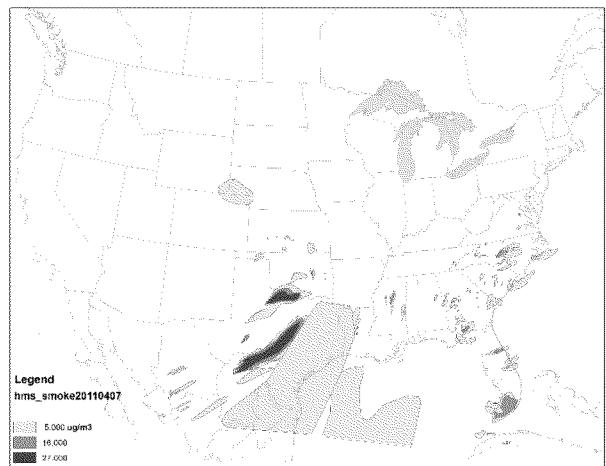
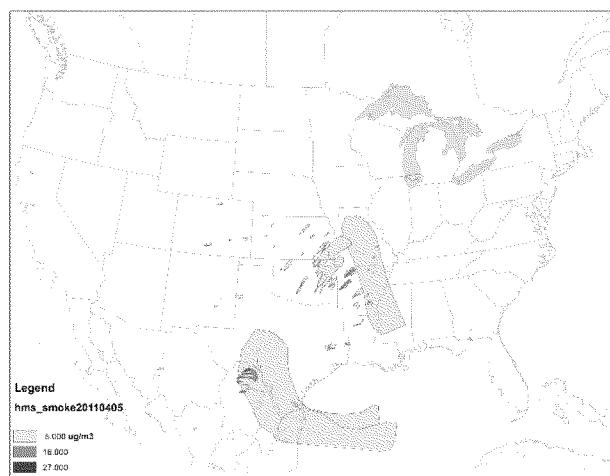
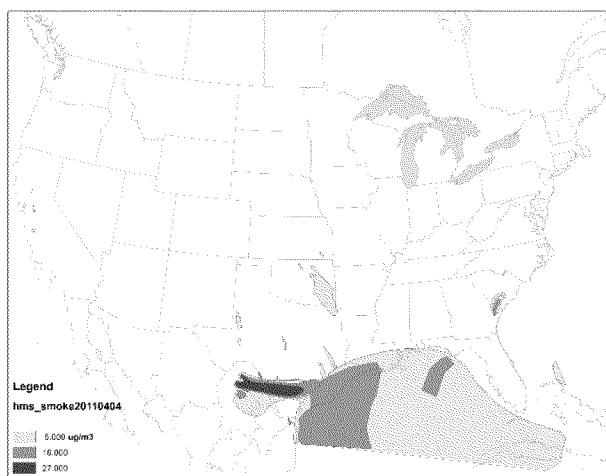
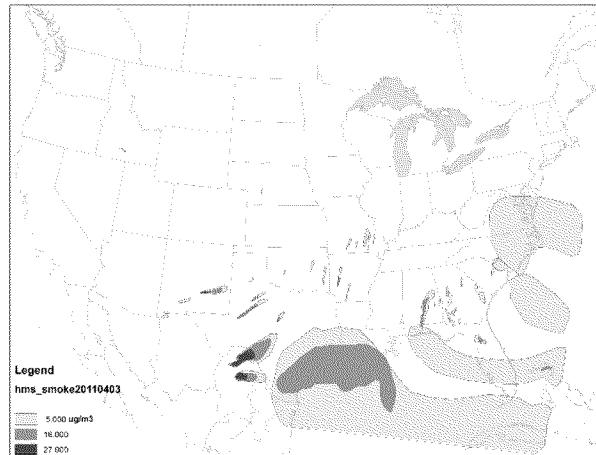
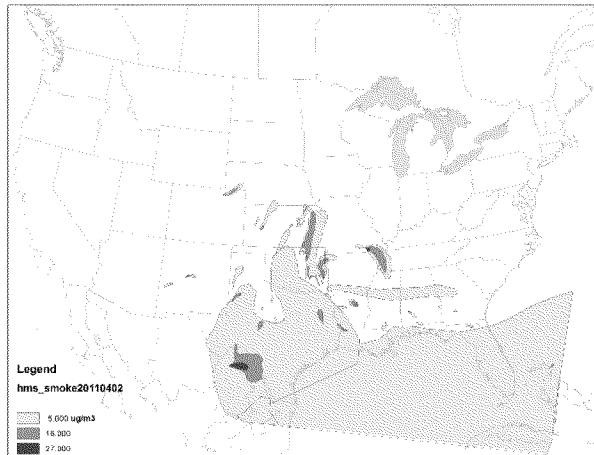


Figure S-4. HMS plots for the Flint Hills fire modeling period in April 2011. The HMS product is a column total smoke density and does not provide an estimate of surface layer O<sub>3</sub> or PM<sub>2.5</sub>.



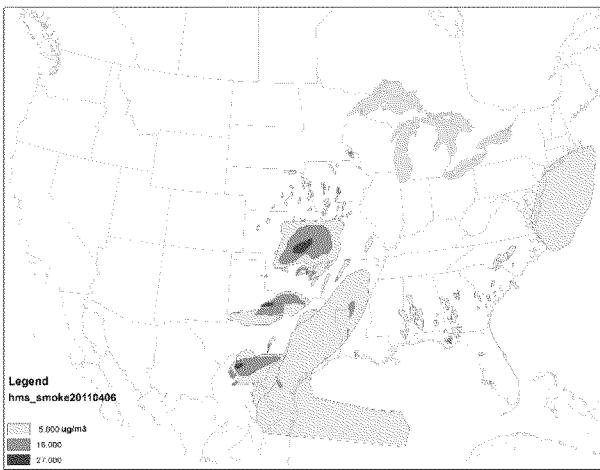
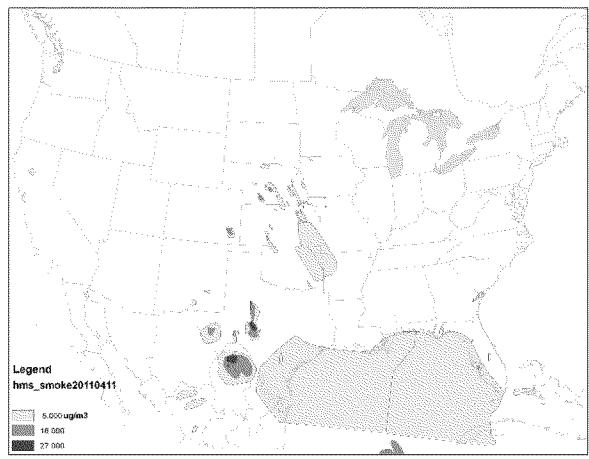
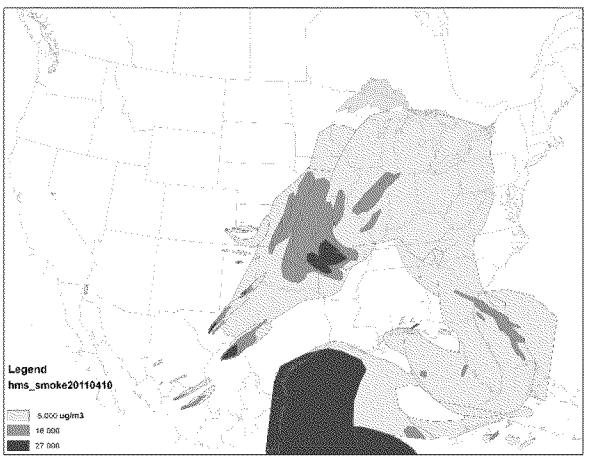
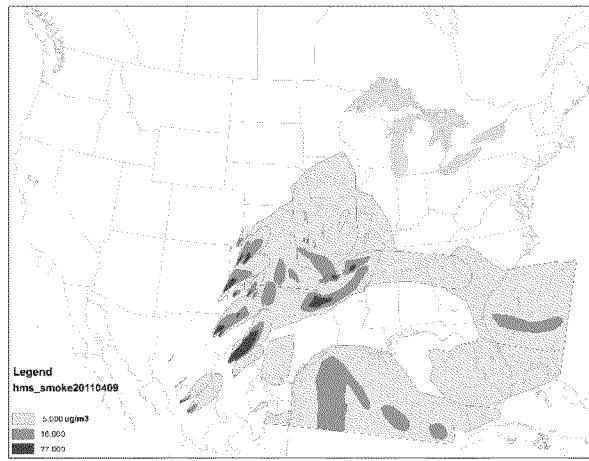
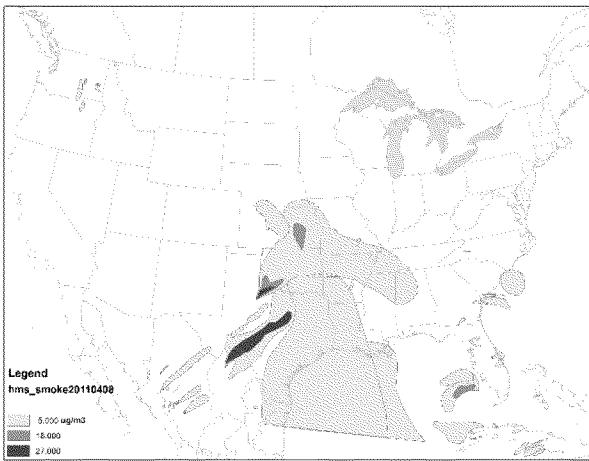
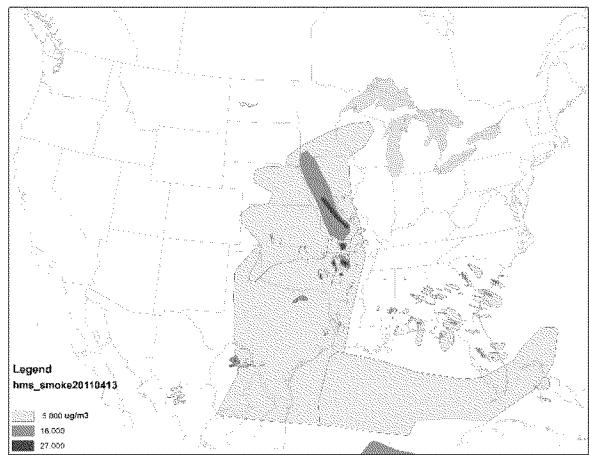
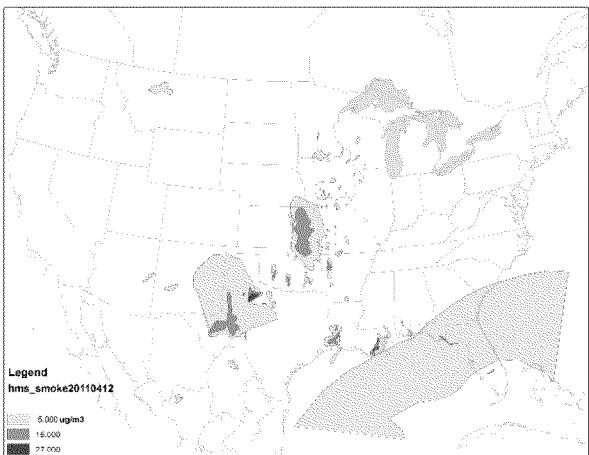


Figure S-4 continued. HMS plots for the Flint Hills fire modeling period in April 2011. The HMS product is a column total smoke density and does not provide an estimate of surface layer O<sub>3</sub> or PM<sub>2.5</sub>.





**Figure S-5. Maximum hourly contribution using ISAM and brute-force zero out for the Wallow fire event.**  
 Contributions shown for CO, precursor gases ( $\text{NO}_x$ ,  $\text{SO}_2$ ,  $\text{NH}_3$ ), primarily emitted  $\text{PM}_{2.5}$  species (EC and POA), and secondary pollutants ( $\text{O}_3$ ,  $\text{PM}_{2.5}$  sulfate ion,  $\text{PM}_{2.5}$  nitrate ion).

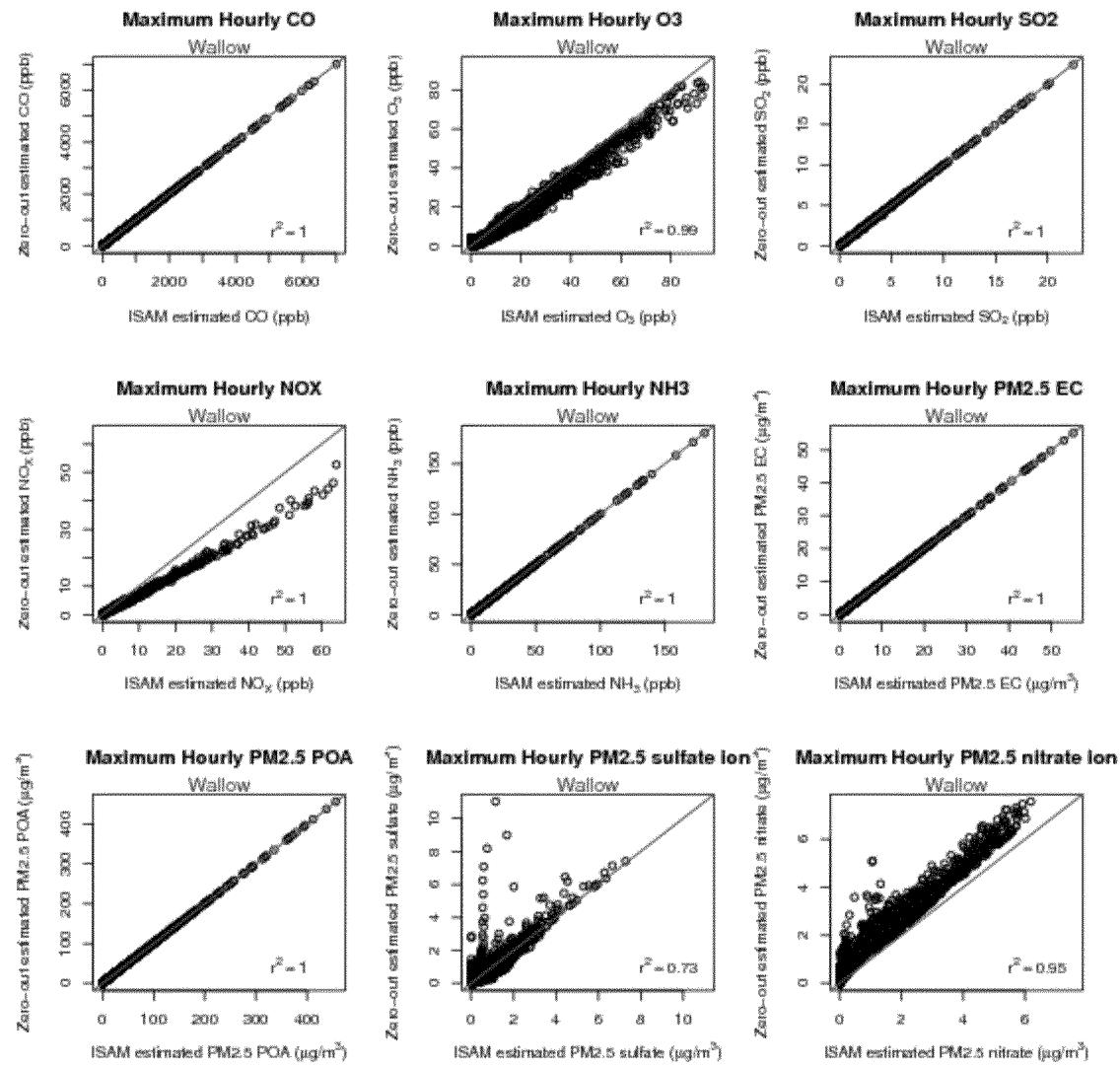


Figure S-6. Maximum hourly contribution using ISAM and brute-force zero out for the Flint Hills fire event. Contributions shown for CO, precursor gases ( $\text{NO}_x$ ,  $\text{SO}_2$ ,  $\text{NH}_3$ ), primarily emitted PM<sub>2.5</sub> species (EC and POA), and secondary pollutants ( $\text{O}_3$ , PM<sub>2.5</sub> sulfate ion, PM<sub>2.5</sub> nitrate ion).

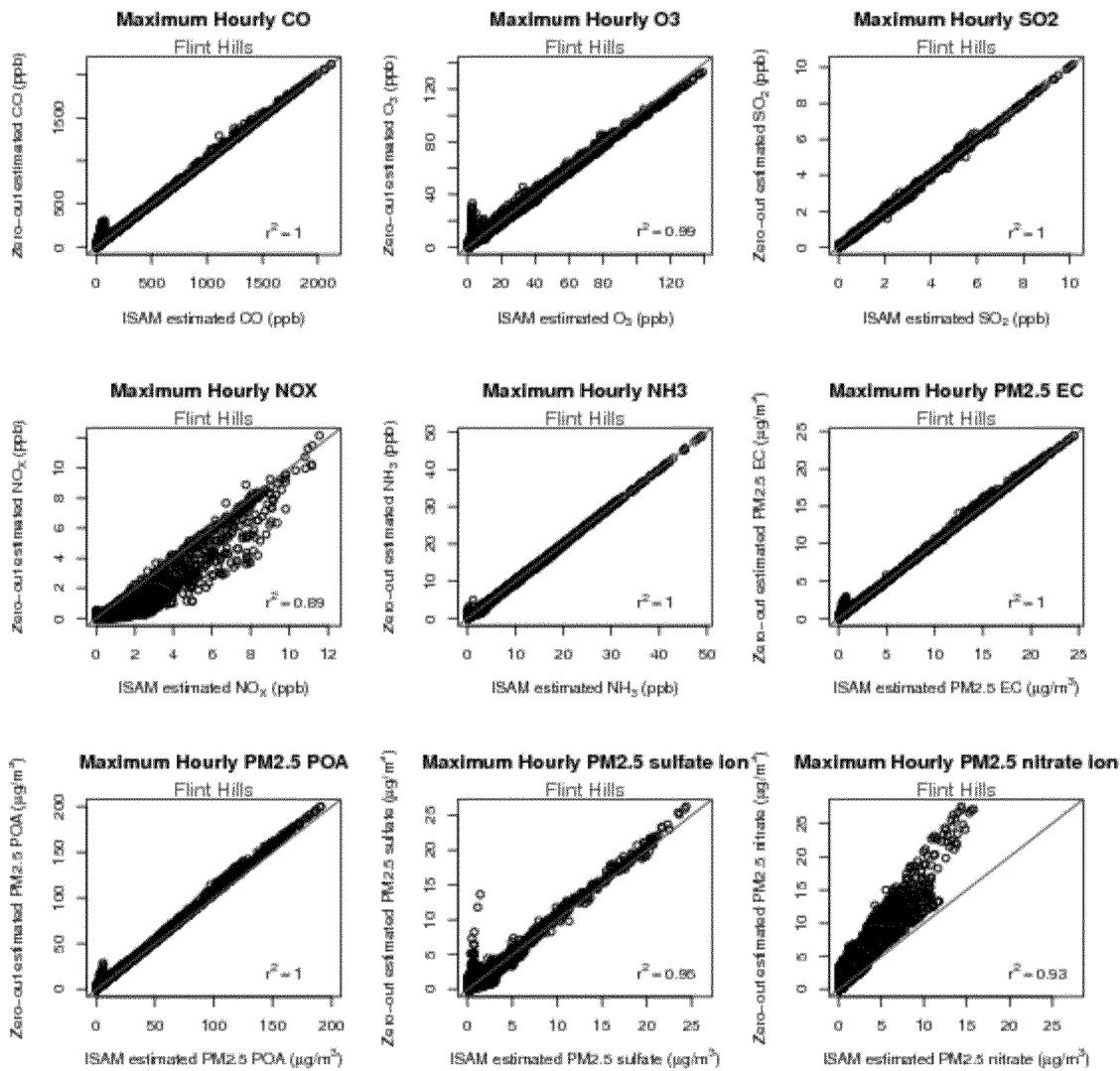


Figure S-7. Maximum hourly contribution using ISAM and brute-force (BF) zero out for the Wallow fire event. Contributions shown for O<sub>3</sub>, NO<sub>x</sub>, and PM<sub>2.5</sub> nitrate ion for each approach and also the difference between approaches. Warm colors indicate the brute-force approach resulted in higher contribution. Cool colors indicate the source apportionment approach resulted in higher contribution.

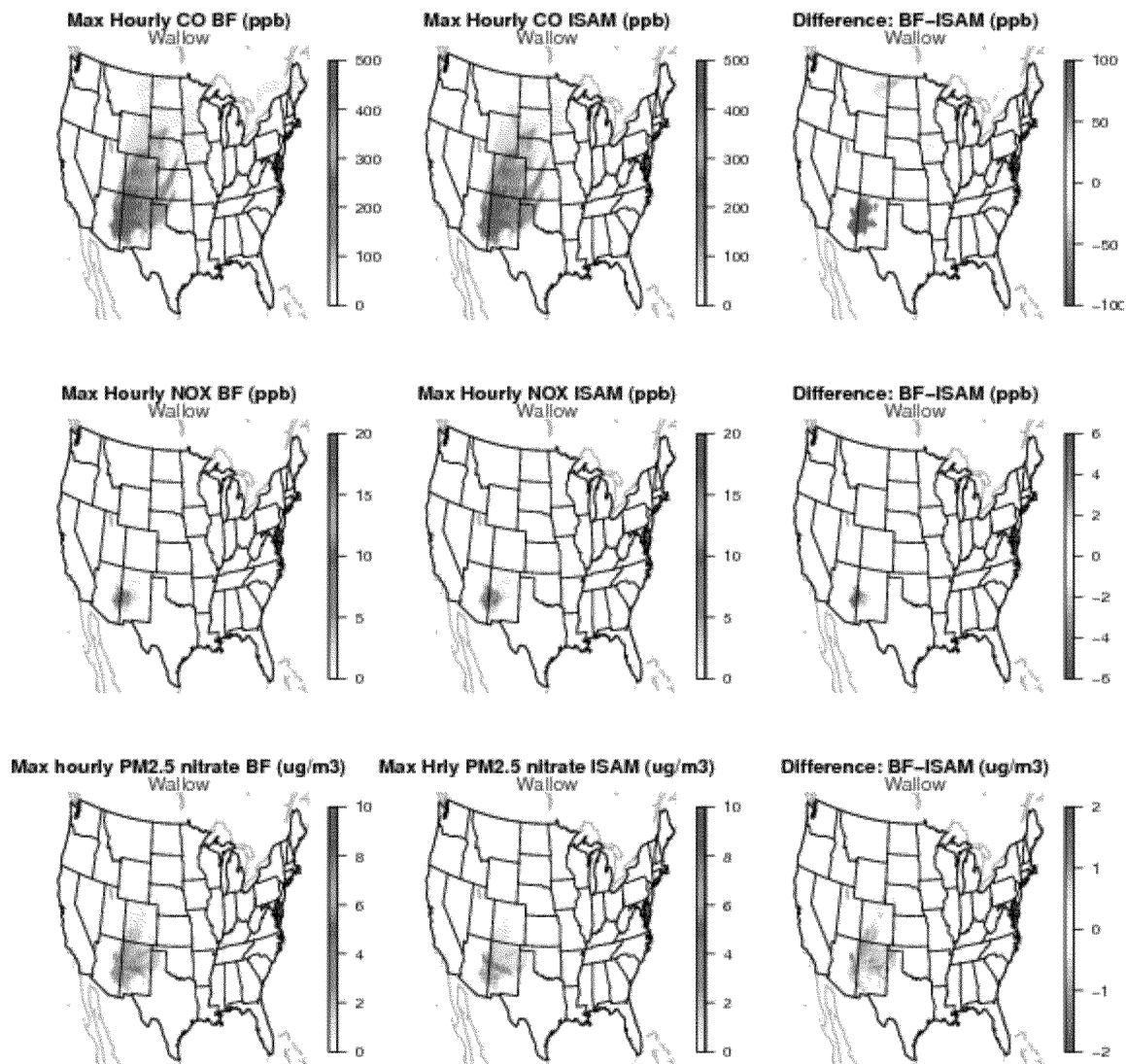


Figure S-8. Maximum hourly contribution using ISAM and brute-force (BF) zero out for the Flint Hills fire event. Contributions shown for O<sub>3</sub>, NO<sub>x</sub>, and PM<sub>2.5</sub> nitrate ion for each approach and also the difference between approaches. Warm colors indicate the brute-force approach resulted in higher contribution. Cool colors indicate the source apportionment approach resulted in higher contribution.

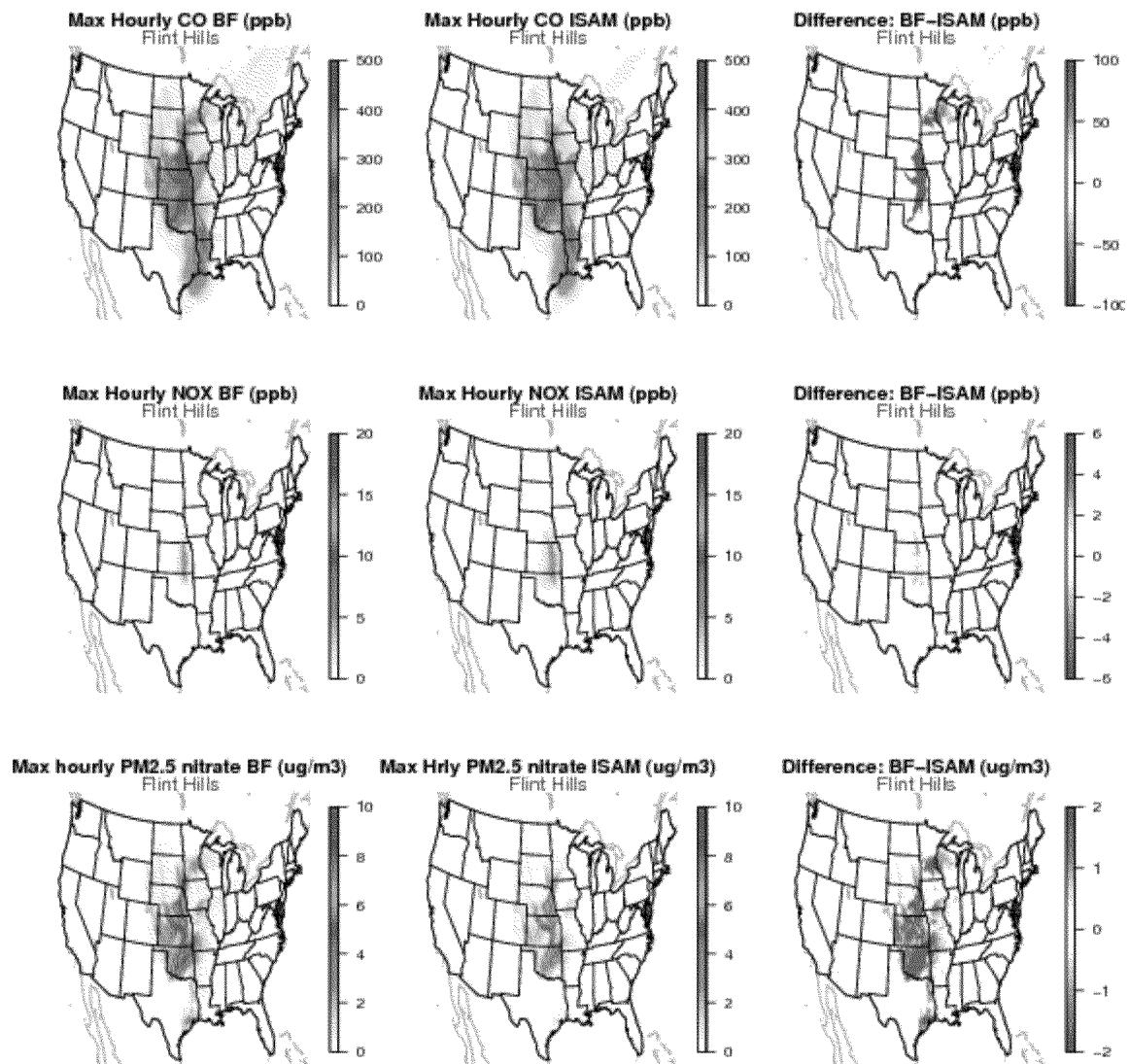


Figure S-9. HCHO production from 11 am to noon for June 4 and 5th for the scenario where Wallow fire emissions are zeroed-out (top row panels). The increase in HCHO and other aldehydes are shown for June 6 at 6 am (middle) and noon (bottom) local time. All results are surface level.

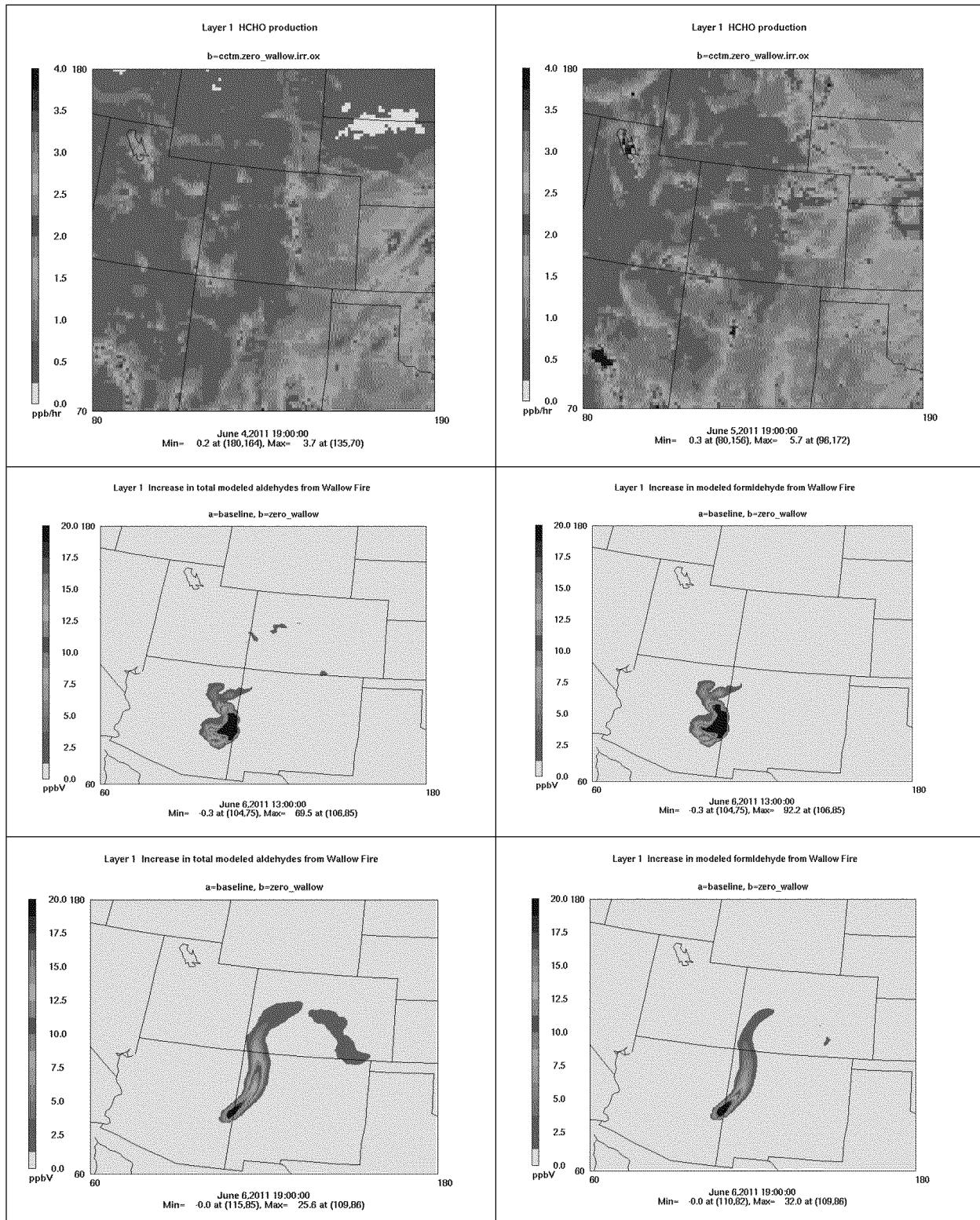


Figure S-10. Maximum hourly impacts from Wallow (top row) and Flint Hills (bottom row) fires to O<sub>3</sub>. The difference between the baseline simulation and sensitivity with reduced photolysis is also shown. Cool colors indicate less O<sub>3</sub> contribution with the sensitivity simulation.

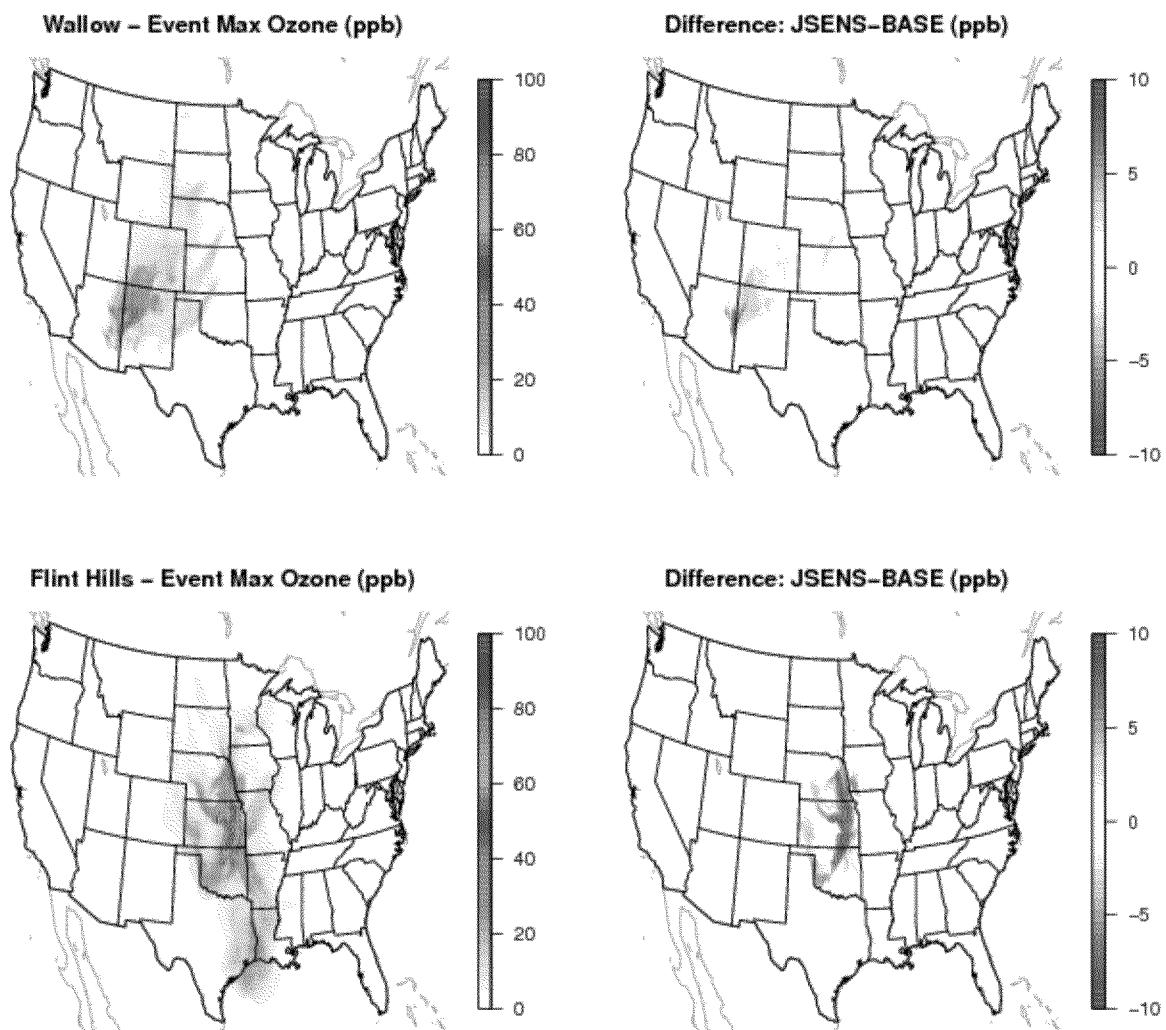


Figure S-11. Hourly PM<sub>2.5</sub> OA enhancement ratios with respect to CO by distance for AE6 and VBS approaches for both fires. The distribution of EC, OA, POA, and SOA are also shown with respect to CO.

